A Sweet Reaction

New understanding of enzyme XI may improve production of biofuel and food products

Recent studies done at Los Alamos on an enzyme that turns one type of sugar into another have yielded some unexpected insights into the reaction.

The enzyme xylose isomerase (XI) can convert the sugar glucose into fructose and is used in manufacturing high-fructose corn syrup for food products. Similarly, XI can convert the sugar xylose into xylulose, which can be used in producing different kinds of biofuels. Understanding those conversion reactions in detail may aid efforts to make the enzyme work better and hence contribute to more-efficient production of fuel and food products.

Xylose has five carbon atoms and one oxygen atom bonded into a hexameric ring, with several hydrogens and hydrogen-oxygen pairs dressing the carbons. To convert from xylose to xylulose, the enzyme helps the ring to open and then helps move two hydrogen atoms from the second to the first carbon in the now-linear molecule.

Researchers from Fox Chase Center, the University of Toledo, the University of Tennessee, and Los Alamos used the Bioscience Division's Protein Crystallography Station (PCS) for their studies. They collected neutrons diffracted from a crystal of XI that had been soaked in a solution of xylose and that the enzyme had converted to xylulose. The neutron crystallographic data revealed the location and charge states (positive or negative charges) of atoms in the XI-xylulose complex. When the results were compared with the team's studies of XI alone, it became possible to see how the atoms had been rearranged during the reaction.

In particular, the researchers discovered that a water molecule held in the active site of XI loses a hydrogen, whereas the enzyme itself acquires one during the shuffling of atoms. The finding, which suggests the water may play some role in the conversion reaction, may help researchers differentiate among several possible reaction mechanisms.

Paul Langan, who built the PCS with Benno Schoenborn, led the Los Alamos team, which also included Andrey Kovalevsky, Marat Mustyakimov, and S. Zoe Fisher. The work was published as a Rapid Report in the journal Biochemistry (Vol. 47, p. 7595, 2008) and listed as a "Hot" article.